A Spatial Kinetic Coupling Scheme Between Two Distinct Turbulence Codes With Minimal Data Exchange

SIAM Annual Meeting (AN18)

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Plan

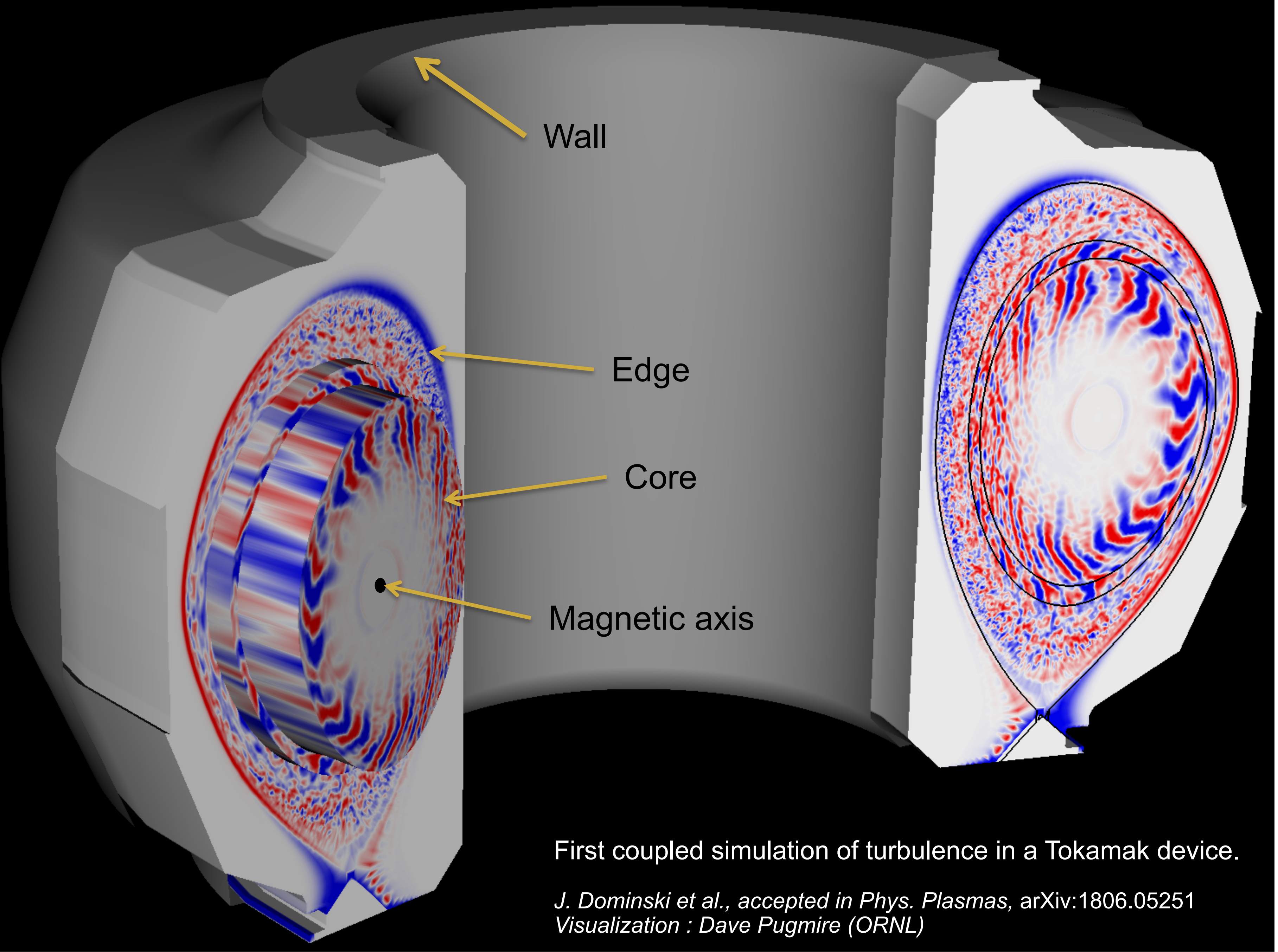
1. **Introduction**
   - Motivation for coupling core and edge gyrokinetic codes
   - The gyrokinetic codes GEM (core), GENE (core), and XGC (edge)

2. **A model for coupling two gyrokinetic simulations,** [J. Dominski, et al., Accepted in Phys. Plasmas] , *arXiv:1806.05251*
   - Coupling model with minimal data exchange
   - Verification of the coupling model with XGC-XGC

3. **Coupling the gyrokinetic codes GENE and XGC together**
   - Interpolation between GENE and XGC grid data
   - Verification of coupled GENE-XGC simulations

4. **Conclusion and perspectives**

Motivation: A High-Fidelity Whole Device Modeling Framework



First coupled simulation of turbulence in a Tokamak device.

J. Dominski et al., accepted in Phys. Plasmas, arXiv:1806.05251
Visualization : Dave Pugmire (ORNL)

Coupling of core and edge codes

1. Core and edge physics are different (different magnetic field topology), even though they use the same equations. Different discretizations are used.
2. Simulation of turbulence physics based on first-principles based 5D kinetic codes (gyrokinetic).
3. XGC is the leading gyrokinetic code for simulating edge region.
4. GEM, GENE, and ORB5 are leading gyrokinetic codes for simulating core region.

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Gyrokinetic codes

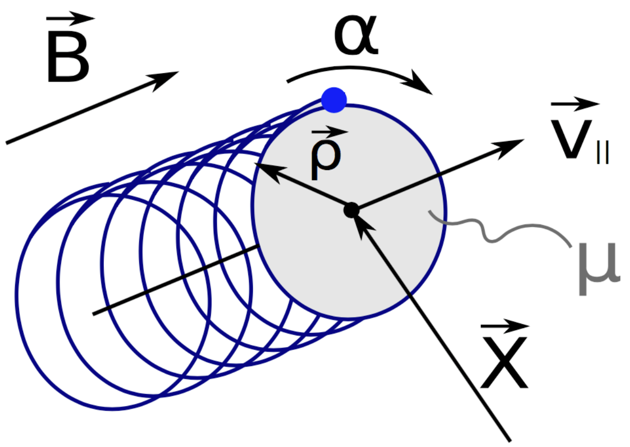
GEM (core)	GENE (core)	XGC (edge)
Particle-In-Cell	Eulerian Grid-based code	Particle-In-Cell
Configuration space: 3D structured rectangular mesh.	Configuration space: structured rectangular mesh in 2 directions and Fourier in the 3rd.	Configuration space: 2D unstructured triangular + 1D structured rectangular mesh.
No grid	Velocity space: adaptive structured rectangular mesh	
Optimized for near equilibrium plasma in **Core**, inside and away from separatrix		Optimized for non-equilibrium plasma in **Edge**
Delta-f perturbation plasma with scale separation		Total-f plasma w/o scale separation
Simulates plasma only without neutrals		Includes wall-interaction, neutrals, atomic physics

2. Model for coupling two gyrokinetic simulations, with minimal data transfer

We have implemented the simplest coupling scheme which only requires the transfer of 3D fields between the core and edge simulations for their coupling.

[J. Dominski et al., Accepted in Phys. of Plasmas] , arXiv:1806.05251

Gyrokinetic equation



Gyromotion is much faster than physics of interest.

Analytical reduction of the gyromotion: 6D => 5D.

The particle distribution function, f, is evolved with the 5D gyrokinetic Vlasov equation

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \dot{\boldsymbol{X}}[\phi] \cdot \frac{\partial f}{\partial \boldsymbol{X}} + \dot{v}_{\|}[\phi]\frac{\partial f}{\partial v_{\|}} = 0, \qquad [1]$$

and the consistent electrostatic potential is solved with the gyrokinetic Poisson equation

$$\mathcal{L}\phi = \bar{n} \qquad [2]$$

where the source term on the right-hand-side is computed from

$$\bar{n} = \int_{-\infty}^{+\infty} dv_{\|} \int_{0}^{+\infty} d\mu \oint d\alpha\, f(\boldsymbol{x} - \boldsymbol{\rho}, v_{\|}, \mu). \qquad [3]$$

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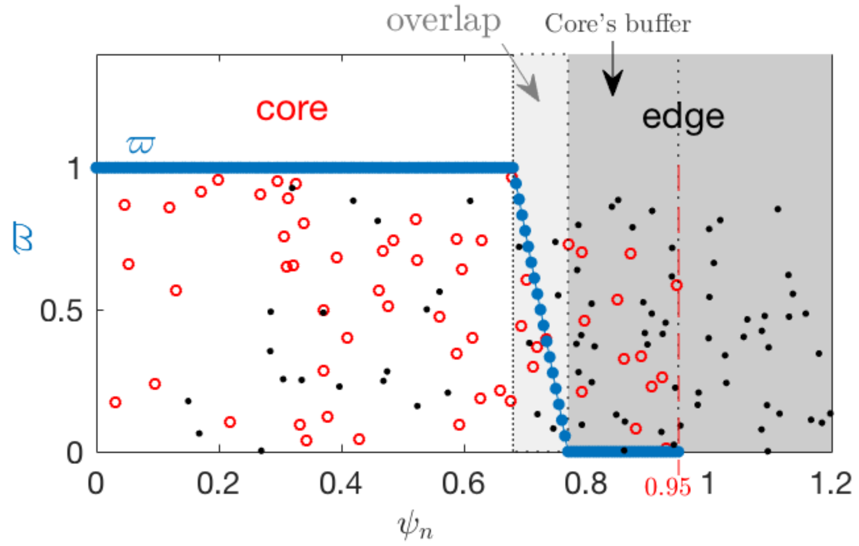
Spatial coupling of gyrokinetic simulations, sharing minimal information

1. In the system of coupled codes, a composite distribution function is used: $f = \varpi f^{Core} + (1-\varpi) f^{Edge}$.

The source term of Poisson Eq. is then computed with

$$\bar{n}[\delta\check{f}] = \int d\boldsymbol{X} dv_{\|} d\mu d\alpha\, \delta_{gc} \left[\underbrace{\varpi(\boldsymbol{X})\delta f^{\mathrm{C}}}_{\text{local in core}} + \underbrace{(1-\varpi(\boldsymbol{X}))\delta f^{\mathrm{E}}}_{\text{local in edge}} \right]$$
$$= \bar{n}[\varpi\delta f^{\mathrm{C}}] + \bar{n}[(1-\varpi)\delta f^{\mathrm{E}}].$$



2. Poisson solver needs the exchange of the 3D fields ϕ and $\bar{n}$ between two codes, not the 5D f.

3. The same ϕ will be used in gyrokinetic Eq. (1) for advancing f independently.

[J. Dominski, et al., Accepted in Phys. Plasmas] , *arXiv:1806.05251*

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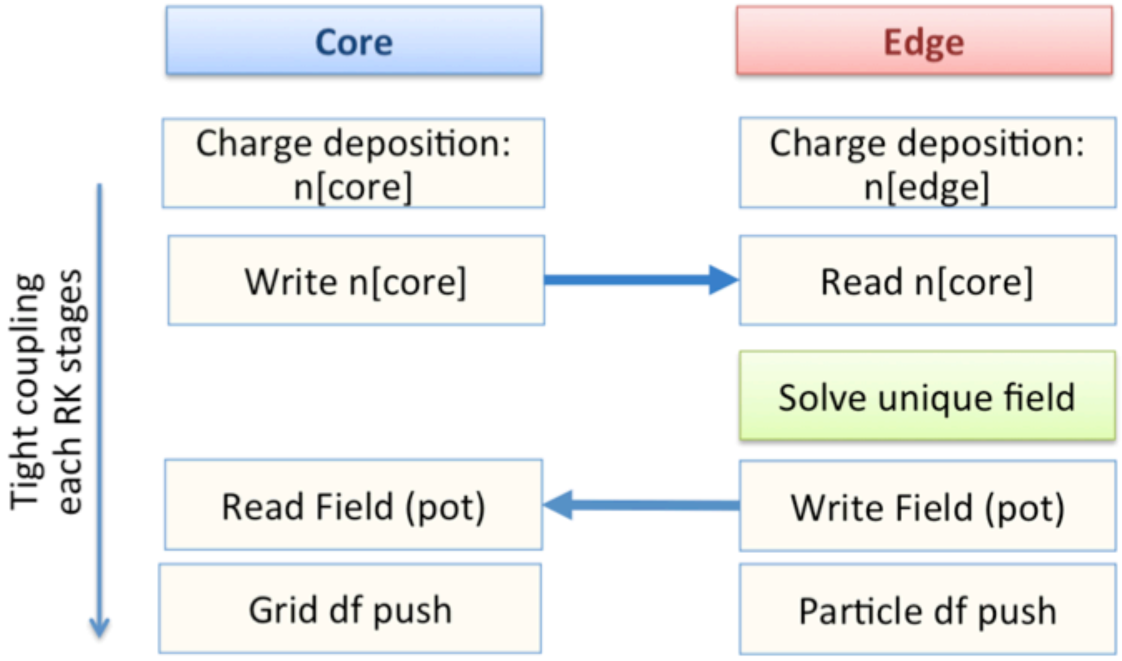
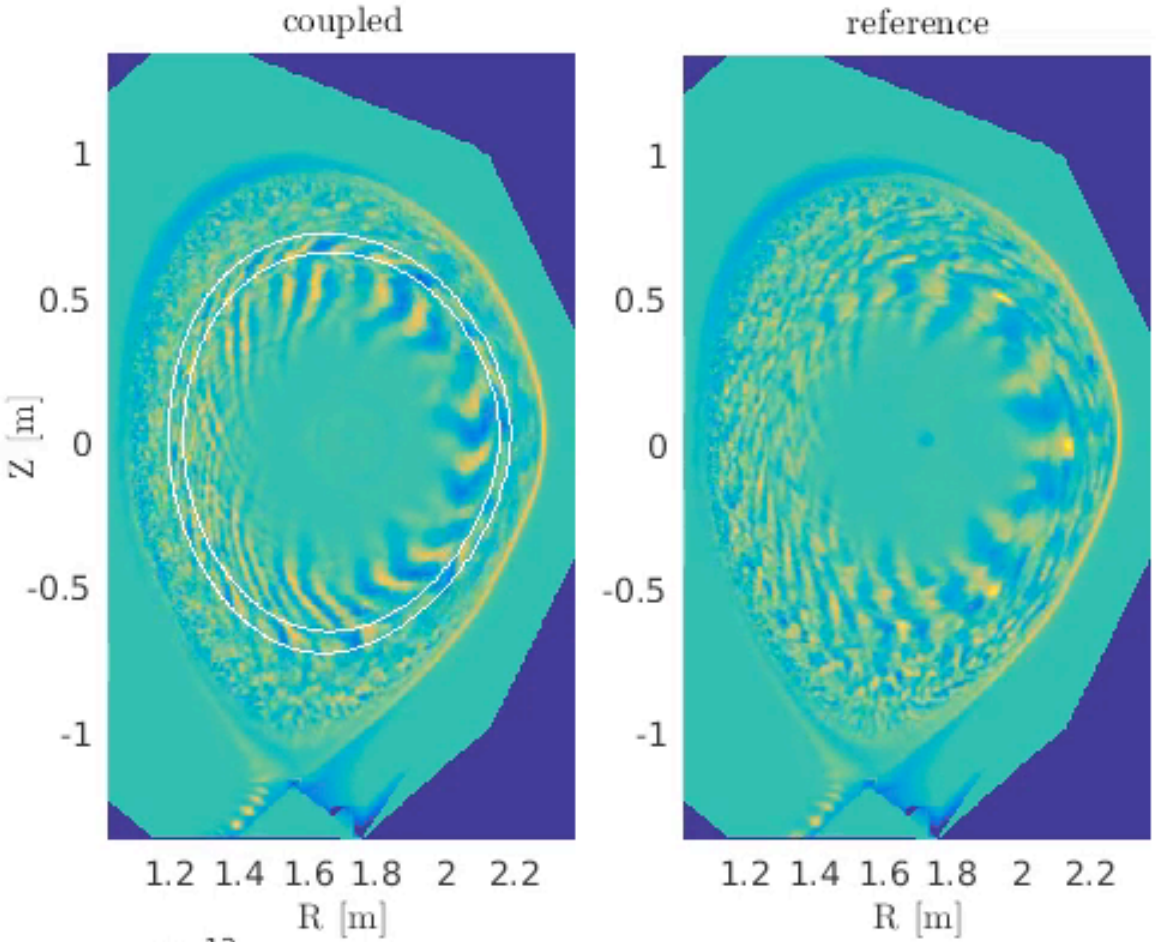
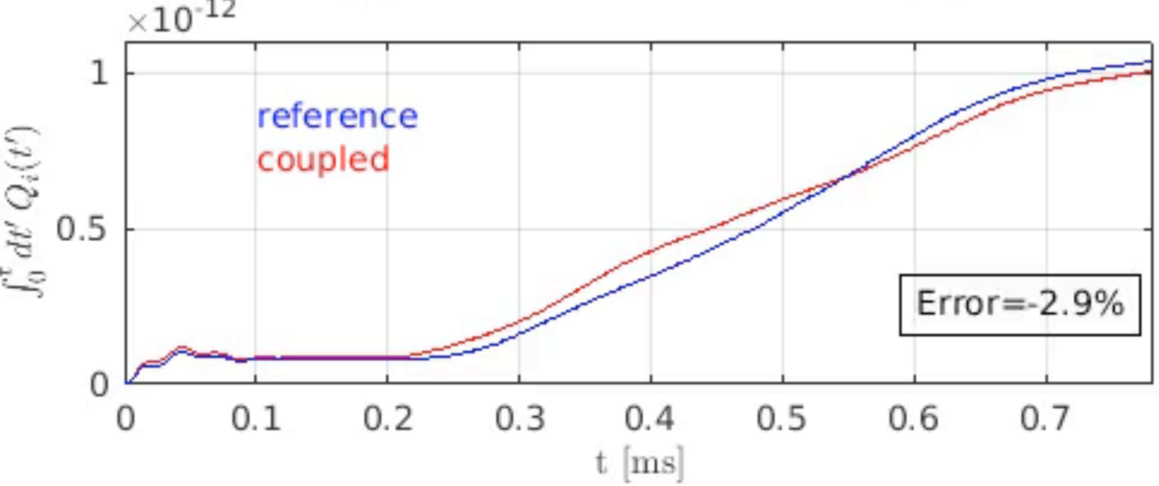
Tight coupling scheme and ADIOS communications

At each stage of the Runge-Kutta time integrator:

1. The core code sends its density contribution to the edge code.
2. The edge code solves the global electrostatic potential.
3. The potential is sent to the core code.
4. Both sides push the Vlasov equation with the same electric field.







Verification of the model

Two XGC executables, one for the core and one for the edge, are coupled together

- It permits to verify the code coupling model without grid interpolation issue.

Test case is a turbulent relaxation problem with realistic geometry and pedestal gradients.

Coupling model has been verified to be accurate within a few percent.

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3. Coupling the gyrokinetic codes GENE and XGC together

We implemented the coupling model verified from the XGC-XGC simulation.

New: the 3D electrostatic potential and density fields have to be interpolated between the structured GENE grid and the unstructured XGC grid.

Interpolation between GENE and XGC grid data

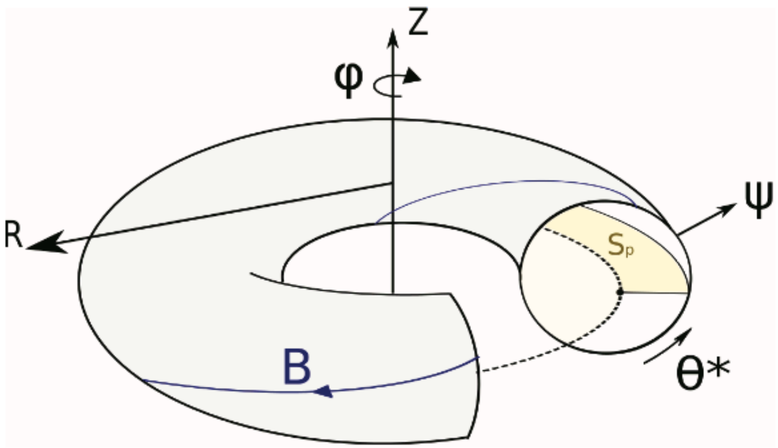
GENE density to XGC grid

$$n(x, k_y, z_{\text{GENE}}) \rightarrow n(x, y, z_{\text{GENE}}) \rightarrow n(x, y, z_{\text{XGC}}) \rightarrow n(R, Z, \varphi)$$

$\rightarrow$ **Field solve** $\rightarrow$

XGC potential to GENE grid

$$\phi(R, Z, \varphi) \rightarrow \phi(x, y, z_{\text{XGC}}) \rightarrow \phi(x, y, z_{\text{GENE}}) \rightarrow \phi(x, k_y, z_{\text{GENE}})$$



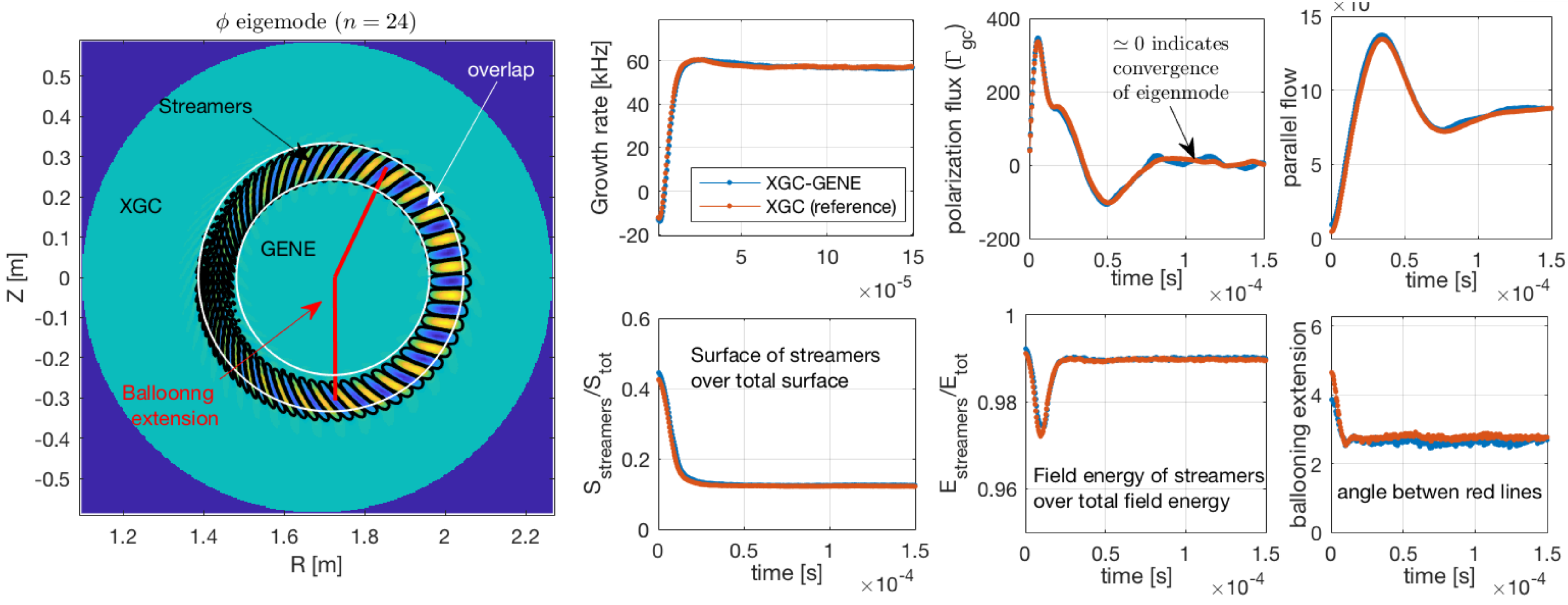
Field-aligned coordinates:

- x = f(ψ)
- y = q θ* - φ
- z = θ*

[G. Merlo, et al., The Sherwood Fusion Theory Conference, Auburn AL, April 2018]

Verification of linear physics in coupled XGC-GENE simulation

A good agreement is found with only a few percent difference.



[J. Dominski et al., Exscale Computing Project meeting, Knoxville TN, March 2018]

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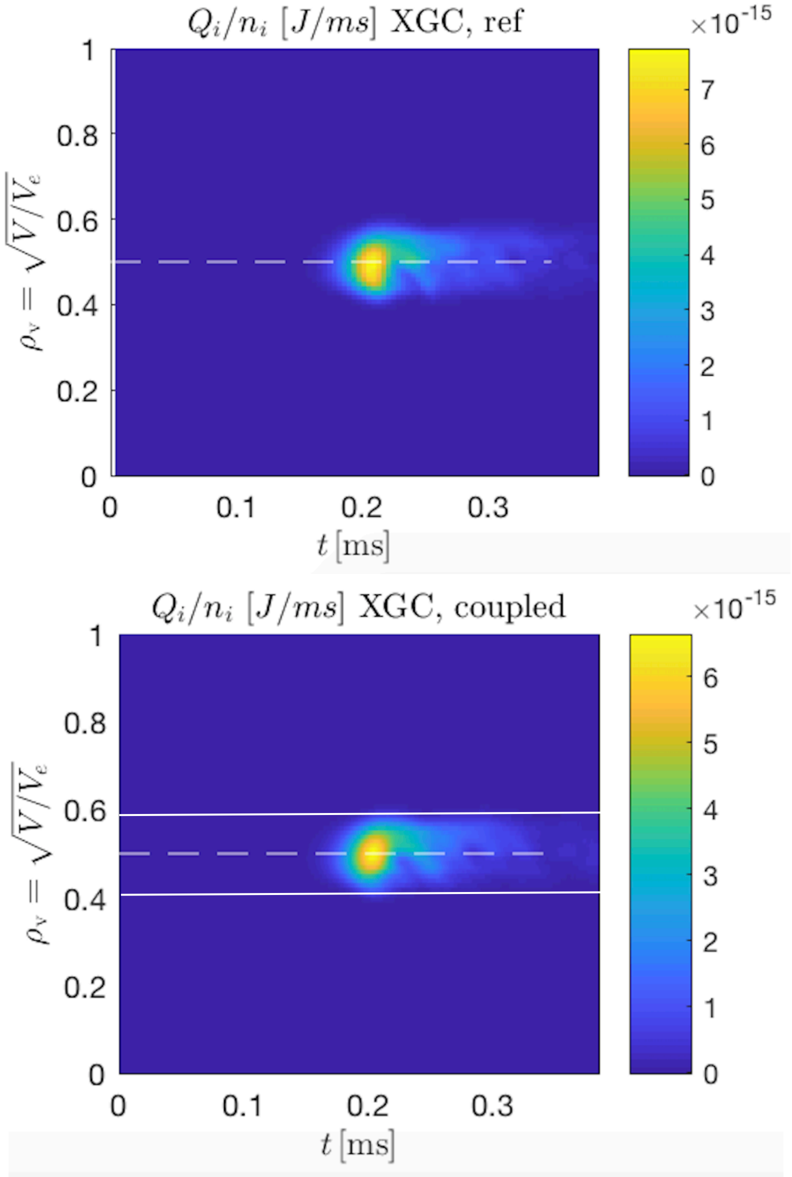
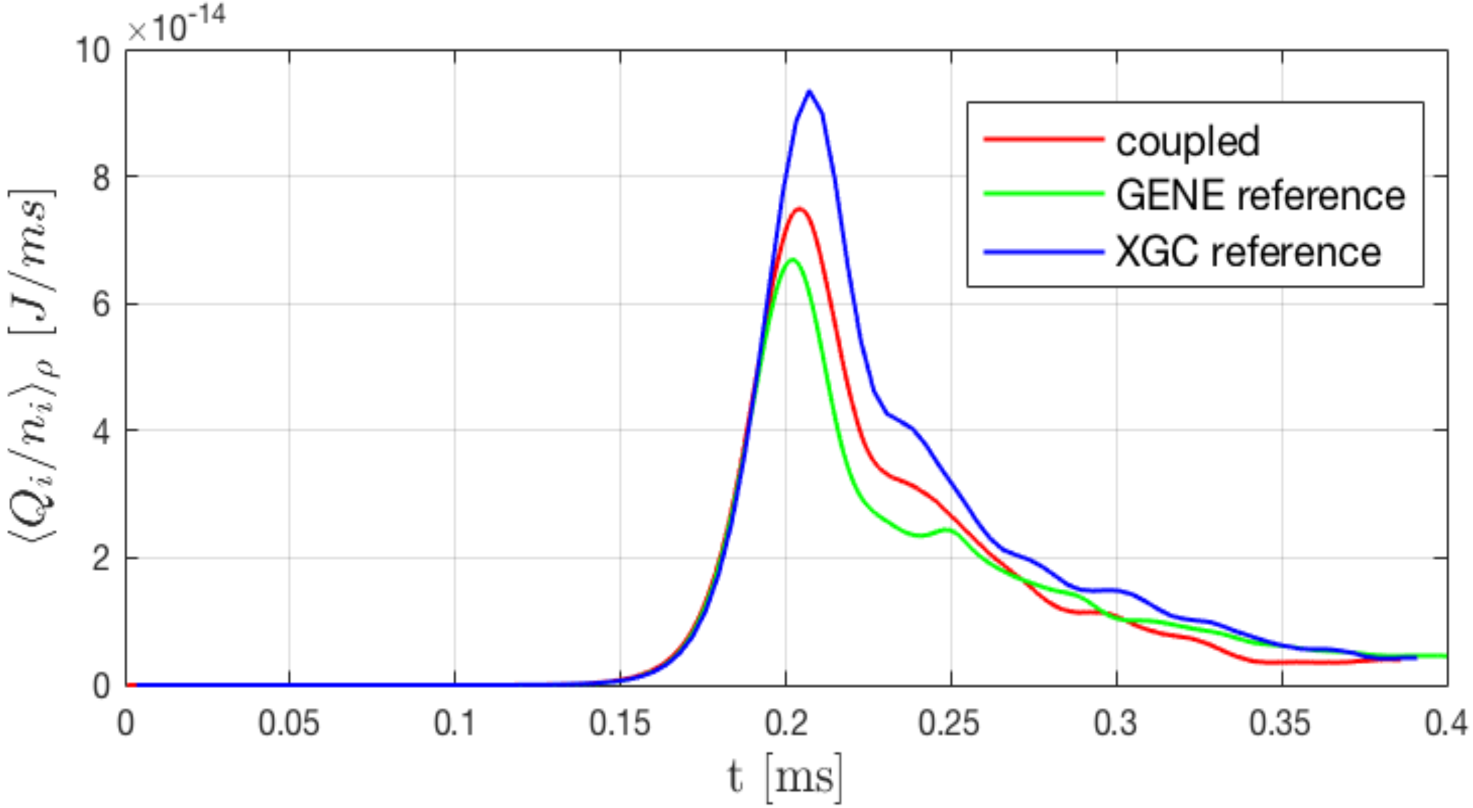
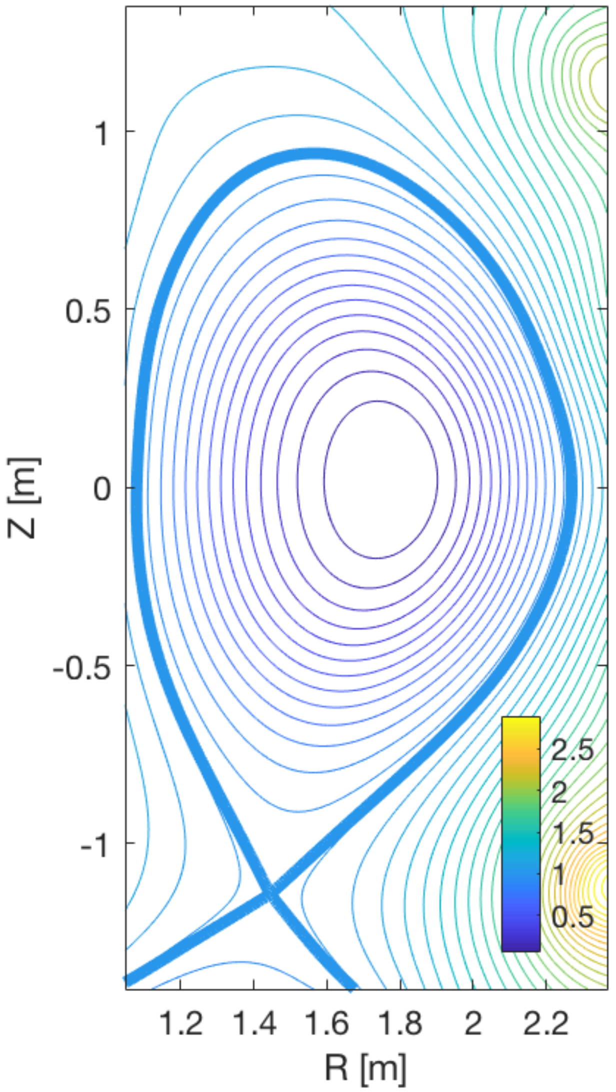
PROJECT

Verification of nonlinear physics in coupled XGC-GENE simulation

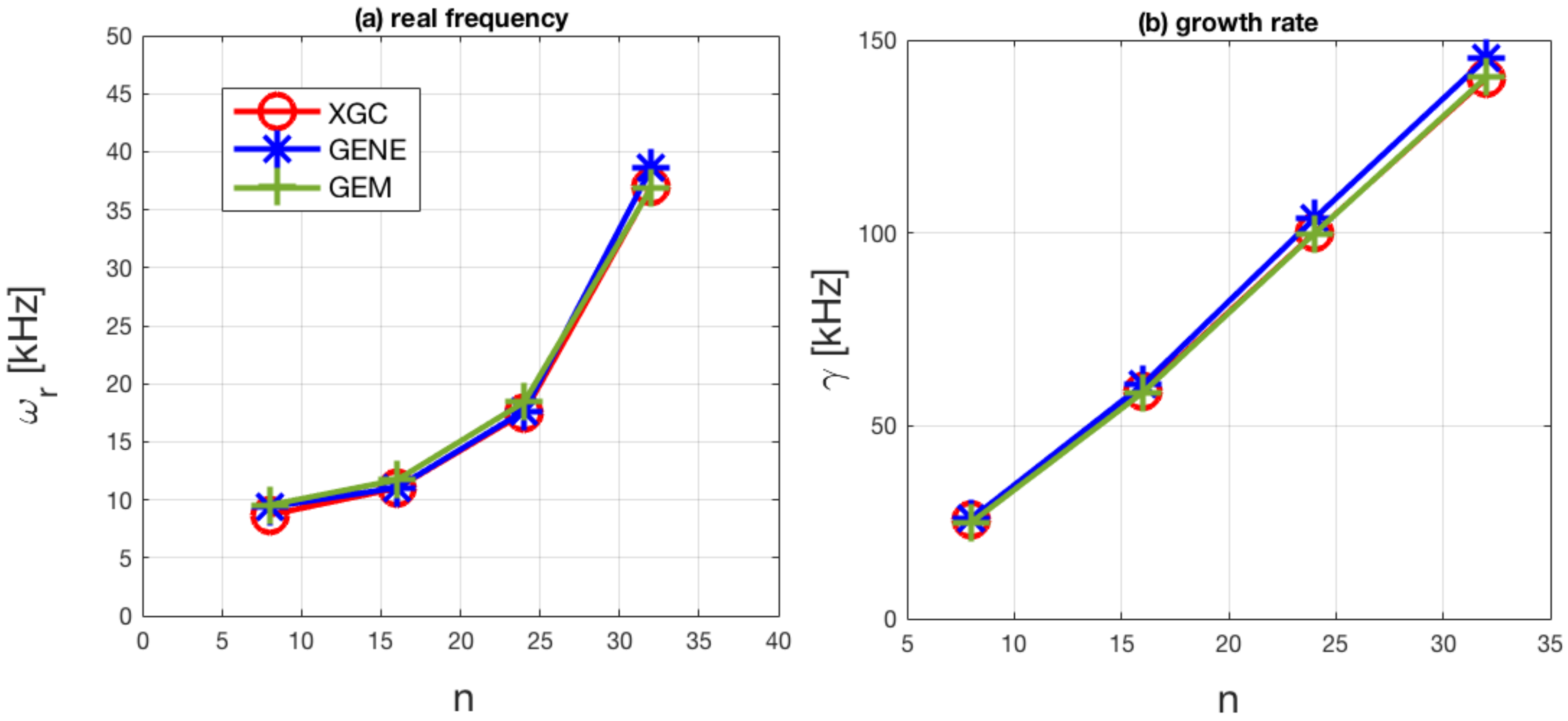




Fully shaped realistic geometry: cross-verification of linear physics

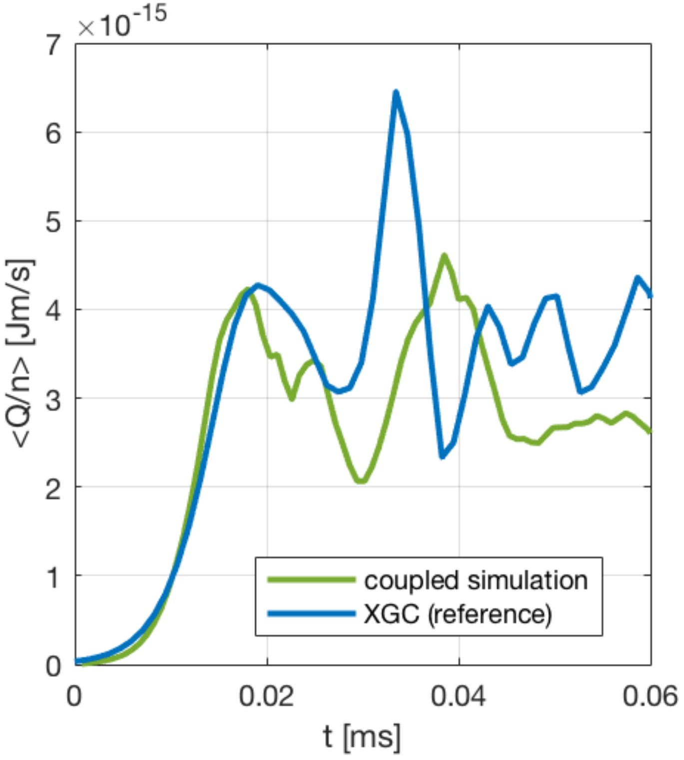


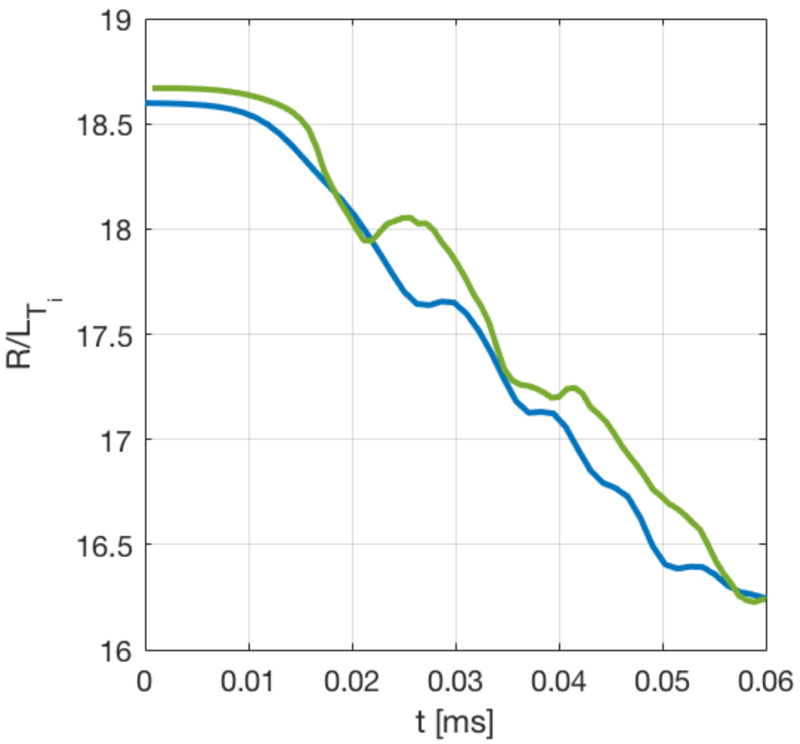
Prior to coupling the codes, we cross-verify the codes. An excellent agreement is found.



Fully shaped geometry: nonlinear physics with the coupled codes

Very good agreement is found between reference and coupled simulation.





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Conclusion and perspectives

- We have a numerical scheme for coupling two gyrokinetic codes with minimal data exchange, well within allowable error bound (experiment).
- We have developed a good technique for grid to grid interpolation.

- Exchange of the 5D f information might be necessary for some other cases. ADIOS is adapted to this kind of massive communication.
- Option of using a particle core code (GEM) could help generalize our coupling approach.